



New class of switchable explosive could revolutionize explosive safety

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This discovery sets the groundwork to revolutionize the safety of explosives

By combining the fields of inorganic coordination chemistry and explosive science, Los Alamos researchers and colleagues from the University of Pennsylvania have documented the very first explosive spin-crossover complex that can transition from a safer “less sensitive phase” to an active “more sensitive phase.” The switching mechanism is reversible with respect to impact sensitivity.

This discovery sets the groundwork to revolutionize the safety of explosives.

“Spin crossover is a property that has been studied for some time, especially in Fe(II) heterocyclic compounds, but no one has reported it in an explosive material nor has anyone correlated it with switchable sensitivity in an explosive,” said Jackie Veauthier of Inorganic Isotope and Actinide Chemistry group.

Spin crossover means the material has two stable electronic spin states (rather than just one) and the material can transition, or switch, between the states. These transitions result in molecular changes (e.g., volume, enthalpy, and bond lengths), which naturally results in one of the states being less sensitive and the other more sensitive. This is an ideal characteristic to hone in explosives.

A spin-crossover material and an explosive

The researchers focused on a particular complex: $[\text{Fe}(\text{Htrz})_3]_n[\text{ClO}_4]_{2n}$. This complex is a known spin-crossover material, but it had not been reported as an explosive. It turns out it's both.

In the current study, the complex's magnetic properties and variable temperature impact sensitivity were measured. For the latter, a new jacketed collar was designed specifically for the test. Density Functional Theory was used to understand how the structural and energy changes that occur upon spin transition correlate to changes in sensitivity. The results indicate that $[\text{Fe}(\text{Htrz})_3]_n[\text{ClO}_4]_{2n}$ is indeed an explosive and, therefore, the first impact-sensitive switchable explosive to be documented.

The spin transition required for the switching mechanism can occur in response to both thermal and non-thermal stimuli, including magnetic fields, pressures, and irradiation

with light. The complex also passed an aging test, which is an indicator of long-term stability.

Beyond this correlation

Spin-crossover materials are popular, and more are being created all the time, mostly for application in electronic devices such as sensors and displays. Many of these inorganic metal coordination spin-crossover complexes have energy-dense, nitrogen-rich ligands that can be derivatized and optimized to have explosive properties. The team is currently working to prepare new samples to be tested as possible switchable explosives.

“The goal is to increase the gap between less sensitive and more sensitive while still being able to switch states, with an ultimate goal of preparing a material that can be switched between an insensitive to a sensitive state,” said Veauthier. This is an ideal method to further enhance the safety of explosives.

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